DBS&A
Daniel B. Stephens & Associates, Inc.

Memorandum

To: Travis Hurst, CRC

Date: December 19, 2022

From: Chris Wolf, P.G. and Beth Salvas, P.G.

Subject: 26R Geochemical Modeling

1. Introduction

For a proposed carbon sequestration project in the Elk Hills Oil Field, CRC has requested that Daniel B. Stephens & Associates, Inc. (DBS&A) perform geochemical modeling to help understand chemical reactions during carbon dioxide (CO_2) storage in the Monterey Formation. Information used to perform the modeling described in this memorandum was obtained from the CRC Class VI permit application materials and other data provided by CRC.

Geochemical modeling was conducted to evaluate the compatibility of the injectate with groundwater and rocks or sediments composing the aquifer system. The intent of the modeling is to identify the major potential reactions that may affect injection or containment (U.S. EPA, 2013).

Geochemical modeling using the PHREEQC (pH-REdox-Equilibrium) software was used to calculate the behavior of minerals and changes in aqueous chemistry based on chemical equilibrium conditions (Parkhurst and Appelo, 2013).

2. Geochemistry for Elk Hills 26R Storage Project

Two geologic units were considered during this evaluation:

- Monterey Formation: Injection reservoir
- Reef Ridge Shale: Sealing unit

The Monterey Formation consists of turbidite deposited sands, and is predominantly composed of quartz and feldspar minerals. The Reef Ridge Shale consists of marine deposited silty or sandy shale and occasional clay beds. While rocks are buried in the earth's crust, chemical reactions between the rocks and groundwater are termed diagenesis, which involves the dissolution of minerals into groundwater and precipitation of minerals from solution. Reactions are driven by fluid movement, temperature, and pressure changes due to burial depth and compaction. Over time, minerals and cements may dissolve and form new minerals. Important reactions that have occurred in the Monterey Formation include the following:

- Precipitation and dissolution of cements and authigenic minerals, consisting of various minerals including quartz, clays, potassium feldspar (K-feldspar), plagioclase feldspar, siderite, gypsum, and pyrite
- Dissolution of feldspars, quartz, lithic fragments
- Formation of feldspar and quartz overgrowths
- Precipitation of illite, kaolinite and other clays

2.1 Monterey Formation Fluid Geochemistry

Data from a water sample from the Monterey Formation were provided (Table 1). The sample results include a complete suite of major ions and pH, so they were used for the geochemical modeling. With a calculated total dissolved solids (TDS) concentration greater than 24,000 parts per million (ppm), the Monterey groundwater is considered brackish.

The net charge of a water sample may be calculated using the cation and anion analytical results. Because water has a net neutral charge, the sum of the cation and anion charges should be zero. Variations due to sampling and analyses often cause the calculated value to vary, and a value within 5 percent of neutral is considered a “good” balance. The charge balance for the sample was calculated in PHREEQC at –0.20 percent.

2.2 Monterey Formation and Reef Ridge Shale Mineralogy

Mineralogy for the Monterey Formation was evaluated using x-ray diffraction (XRD) to determine the bulk and clay mineralogy of core samples. The Monterey Formation consists of turbidite sands, and is composed predominantly of quartz and feldspar minerals (Table 2). The amount of clay minerals varies from 8 to 26 percent, and they are mostly illite and smectite minerals.

Mineralogy for the Reef Ridge Shale was evaluated using Fourier transform infrared spectroscopy (FTIR) to determine the bulk and clay mineralogy of core samples. The Reef Ridge Shale consists of silty or sandy shale, and the mineralogy identified by FTIR is typically dominated by the Opal-CT quartz mineral and layered illite and smectite clay minerals. Based on the FTIR analyses, 5 to 46 percent of the formation consists of clay minerals (Table 3).

2.3 Injectate Chemistry

For the geochemical modeling, two scenarios of different chemical compositions for the carbon dioxide injectate were developed (Table 4). The compositions were normalized to 100 percent for use as model input. For Scenario 2, the ethane component was excluded from the geochemical analysis because ethane gas is not in the model database. The normalized chemistry for Scenario 1 and Scenario 2 was modeled at 26R.

3. Equilibrium Geochemical Modeling

When modeling groundwater geochemistry, the water chemistry, gas chemistry, and mineralogy are used to constrain the model because mineral solubility controls the concentrations of its components in groundwater (Appelo and Postma, 2005). Mineral dissolution-precipitation reactions directly impact the aqueous chemistry. In general, as minerals dissolve, the concentrations in groundwater increase and when minerals precipitate, the concentrations in groundwater decrease. Chemical equilibrium indicates that congruent reactions will appear balanced between reactants and products, with no apparent change in the chemical system.

The PHREEQC model was used to evaluate potential changes to mineralogy and aqueous composition in the subsurface due to carbon dioxide injection. The mineral, gas, and aqueous phases were assumed to be in chemical equilibrium.

Based on the available injectate gas compositions, the ideal gas law and Raoult's Law were used to calculate the gas composition in moles. The initial and final pressures of 23.1 and 222.1 atmospheres (atm), respectively, were used to calculate the partial pressures of the injectate components.

A reservoir temperature of 99°C was used for 26R.

3.1 Geochemical Database

For reactions involving water and minerals, the equilibrium relationship between products and reactant activities (concentrations) can be calculated using known values for parameters like Gibb's energy found in thermodynamic databases (Zhu and Anderson, 2002). Thermodynamic values for these calculations are compiled in databases from several entities including the

U.S. Geological Survey (USGS) and Lawrence Livermore National Laboratory. A database developed at the Lawrence Livermore National Laboratory (LLNL.dat) was used for this evaluation. The LLNL.dat database includes a temperature range for the thermodynamic data provided from 0 to 300°C. This database is appropriate for the groundwater concentrations, pressure, and temperature used in the modeled scenarios.

When modeling saline waters, the Pitzer database (Parkhurst and Appelo, 2013) is often used, but it has thermodynamic data for a limited number of minerals including calcite, dolomite, gypsum, and quartz. The Monterey Formation and Reef Ridge Shale are predominantly composed of minerals that are not included in the Pitzer database, so the LLNL.dat database was used because it also includes smectite, illite, pyrite, and the minerals listed in Tables 2 and 3.

3.2 Saturation Indices

Saturation indices (SIs) were calculated that represent whether a particular mineral (e.g., calcite) is in chemical equilibrium with the groundwater. SI calculations are used to predict if a mineral is likely to precipitate or dissolve in the groundwater and if these reactions changed the concentrations of dissolved elements.

Chemical equilibrium was assumed for the reactions in the model. Equilibrium modeling sets the saturation indices to a zero (0) value for a given mineral. Minerals used in the modeling scenarios are based on those detected using XRD and their relative abundances. The assumption of chemical equilibrium allows dissolution and precipitation reactions to be quantified in the model.

The formula for calculating saturation indices (SI) is as follows:

$$SI = \frac{IAP}{K_{sp}} \tag{1}$$

where SI = saturation index
IAP = ion activity product
K_{sp} = solubility product

Using gypsum as an example (Clark, 2015), the ion activity product of gypsum (IAP_{gypsum}) is the product of the activity (a, activity is approximately equal to concentration in dilute solutions) of calcium (Ca) and sulfate (SO_4):

$$IAP = a_{Ca^{2+}} \times a_{{SO_4}^{2-}} \tag{2}$$

The solubility product, K_{sp}, is an indication of the relative solubility of a mineral in water. A value less than zero (<0) indicates that the mineral will dissolve and contribute ions to solution and may result in a relatively high activity or concentration. A value greater than zero (>0) indicates that the mineral has a low solubility, may precipitate from solution, and will not contribute many ions to the solution. For the mineral gypsum, the K_{sp} based on the dissociation reaction of gypsum in water is:

$$CaSO_4 \cdot 2H_2O \leftrightarrow Ca^{2+} + SO_4^{2-} + 2H_2O$$

$$K_{sp} = \frac{a_{Ca^{2+}} + a_{SO_4{}^{2-}} + a_{H_2O}}{a_{gypsum}} = 10^{-4.60} \tag{3}$$

Interpreting the results of the SI calculation is straightforward:

- SI > 0 indicates that mineral is supersaturated in solution and may precipitate onto aquifer matrix
- SI = 0 indicates that mineral is at chemical equilibrium with the water
- SI < 0 indicates that mineral is undersaturated in solution and may dissolve from aquifer matrix

Due to potential systematic errors introduced during sampling and analysis, results within the range of ±0.5 of zero are typically considered in or near chemical equilibrium.

4. Geochemical Model Input

To construct the equilibrium models in PHREEQC, site-specific data were used as input, including water chemistry, mineralogy, temperature, and pressure.

Data include the water chemistry for the Monterey Formation (Table 1) that were entered as received in ppm for elemental concentrations and standard units for pH.

In order to model the geochemistry of the clay minerals identified by XRD or FTIR, potassium (K) and aluminum (Al) concentrations were calculated in PHREEQC by equilibrating the provided water chemistry with the aluminosilicate clay mineral, Illite at 99°C and 23.1 atm. The modeled aqueous concentrations were used in subsequent modeling at 0.4 ppm K and 1.07 ppm Al for 26R. These concentrations are reasonable for a sandstone aquifer at the neutral pH values in the Monterey Formation.

For input into PHREEQC model, the mineralogy of the Monterey Formation (Table 2) and of the Reef Ridge Shale (Table 3) were converted to moles per liter (mol/L) using porosity and bulk density values as follows:

- Monterey Formation injection zone at 26R, porosity of 25 percent and rock density of 2.65 kg/L
- Reef Ridge Shale upper confining zone at 26R, porosity of 7 percent and rock density determined for the individual FTIR sample (Table 3)

The converted values for mineralogy that were input into PHREEQC are in shown Tables 5 and 6.

Average temperature provided for the Monterey Formation is 99°C at 26R with an initial average pore volume pressure of 23.1 atm, which is expected to increase to 221.1 atm by project completion. The amount of carbon dioxide in 1 liter of gas at 23.1 atm and 99°C based on ideal gas law (PV = nRT) is 0.758 moles, and the amount of gas in 1 liter increases to 7.244 moles at 221.1 atm.

5. Geochemical Modeling Results and Discussion

Model results showing the changes in mineralogy designated as equilibrium phases in PHREEQC are presented for 26R in Table 7 for the Monterey Formation and in Table 8 for the Reef Ridge Shale. Model results are presented in Table 9 for 26R for the water chemistry based on the equilibrium phases. The modeling steps were as follows:

- Monterey Formation: Use the Monterey groundwater sample and equilibrate with selected mineralogy data set for the Monterey Formation (Table 5) with Scenario 1 injectate chemistry at initial and final reservoir pressures
- Reef Ridge Shale: Use the model results for Monterey 5,981.5 depth at final reservoir pressure and equilibrate with selected Reef Ridge Shale mineralogy data set (Table 6) with Scenario 1 injectate chemistry at final reservoir pressure
- Repeat both steps using the Scenario 2 injectate chemistry

Equilibrium geochemical modeling of the injection of carbon dioxide indicate that changes in mineralogy and aqueous chemistry are likely to occur, but overall, both geologic units are composed dominantly of silicate minerals such as quartz and feldspar that are not expected to be highly reactive during carbon dioxide sequestration. More reactive minerals like calcite and dolomite are present in relatively smaller amounts compared to the silicate minerals.

Although the model indicates minerals will dissolve and precipitate, the net change in mass is minimal. Based on the molar mass, there is a small increase of less than 1.2 percent in the Monterey Formation under Scenario 1, and a small decrease of less than 0.2 percent under Scenario 2. For the Reef Ridge Shale, there is a small molar mass increase of about 1 percent in Scenario 1 and Scenario 2. The amount of porosity in the Monterey Formation and the Reef Ridge Shale is not expected to be significantly impacted by mineral dissolution and precipitation reactions during carbon dioxide sequestration.

The TDS concentration is predicted to increase as dissolved aqueous species increase from the injection gases dissolving into the groundwater.

Based on the modeling, the following reactions are expected to occur in the Monterey Formation:

- Dissolution of feldspars and the precipitation of quartz and siderite.
- Smectite and/or kaolinite dissolution resulting in the precipitation of illite.
- Chlorite (chamosite) when initially present is not stable, and dissolves releasing iron, aluminum and silica to solution.

Based on the modeling, the following reactions are expected to occur in the Reef Ridge Shale:

- Illite dissolution that may contribute magnesium (Mg) for the precipitation of dolomite as well as silica and aluminum that may be at least partially precipitated as other aluminosilicate minerals like k-feldspar.
- Albite and k-feldspar are stable and tend to precipitate removing sodium, silica, aluminum, oxygen, and potassium from solution.
- Pyrite tends to be stable in under both injection scenarios.

For both geologic units, the formation of carbonates like dolomite or siderite was predicted to occur in every model scenario. The formation of carbonate minerals can be an important mechanism to remove and immobilize carbon dioxide from solution through incorporation in the mineral phase.

The CO_2 gas in the injectate will form carbonate minerals, dissolve into solution, or remain in a gas phase.

Based on the equilibrium modeling, the aqueous chemistry results are provided in Table 9. Results indicate the following:

- Carbon dioxide will dissolve into solution, and is included in the total inorganic carbon (TIC), which also includes bicarbonate and carbonate species. Results indicate that when carbon dioxide is dissolved in solution, the following dissolved species will occur as the following ions and complexes: carbon dioxide, bicarbonate, sodium bicarbonate, calcium bicarbonate, and magnesium bicarbonate.
- The pH values ranged from 6.1 to 6.5 in 26R.
- The pe remains negative, indicating reducing conditions.
- The calcium in solution includes the following ions and complexes: calcium, calcium bicarbonate, and calcium sulfate complex.

Based on the geochemical equilibrium modeling, the injection of carbon dioxide at the 26R site into the Monterey Formation does not cause significant reactions that will affect the injection or containment of the gas.

References

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Tables

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Table 1. Baseline Geochemistry, 26R Monterey Formation

Analyte	Concentration (ppm [a]) at 317-26R
Barium	57
Bicarbonate	2,441.8
Calcium	92
Chloride	11,424
Magnesium	19
pH (s.u.)	8.2
Silica	50
Sodium plus potassium	8,775
Sulfate	1,198
Total dissolved solids	24,056.8

[a] Unless otherwise noted
ppm = Parts per million
s.u. = Standard units

Table 2. Mineralogy for the Monterey Formation

Mineral Constituent	Relative Abundance (%)							
Depth (feet)	*5,912.5*	*5981.5* [a]	*6,046.0*	*6,046.9*	*6,066.4*	*6,097.1*	*6,113.3*	*6,141.0*
Bulk Minerals								
Quartz	38	40	40	37	41	41	35	44
K-feldspar	15	16	14	17	18	16	19	6
Plagioclase feldspar	32	32	29	37	32	34	34	17
Siderite	0	0	0	0	0	0	0	3
Pyrite	1	1	2	1	1	0	1	3
Gypsum	1	1	0	Trace	0	0	0	1
Bulk Subtotal	*87*	*90*	*85*	*92*	*92*	*91*	*89*	*74*
Clay Minerals								
Illite/smectite	3.64	2.9	4.8	2.88	2.4	1.71	1.76	19.5
Fe-Illite/mica	8.45	5.6	6.75	3.6	3.28	4.77	5.06	5.72
Kaolinite	0.52	1.1	3	1.2	2.08	2.25	3.63	0.78
Chlorite	0.39	0.4	0.45	0.32	0.24	0.27	0.55	0
Clay Subtotal	*13*	*10*	*15*	*8*	*8*	*9*	*11*	*26*
Sample total	100	100	100	100	100	100	100	100

[a] Most likely mineral composition for Monterey Formation selected for modeling

Table 3. Mineralogy of the Reef Ridge Shale
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Mineral Constituent	Relative Abundance (%)																	
Depth (feet)	*5,285.5*	*5,290.0*	*5291.8* [a]	*5,295.5*	*5,299.2*	*5,299.8*	*5,302.2*	*5,304.2*	*5,308.1*	*5,318.0*	*5,325.0*	*5,333.0*	*5,336.9*	*5,338.8*	*5,341.2*	*5,341.7*	*5,346.1*	*5,350.1*
Density (g/cm^3)	*2.51*	*2.38*	*2.51*	*2.49*	*2.52*	*2.49*	*2.44*	*2.50*	*2.51*	*2.50*	*2.52*	*2.51*	*2.37*	*2.48*	*2.81*	*2.50*	*2.78*	*2.49*
Bulk Minerals																		
Quartz	12	0	0	0	0	0	0	0	0	0	12	10	0	0	0	9	0	13
Opal-CT	26	57	39	42	35	37	39	25	23	34	23	30	63	45	0	34	0	31
Chert	0	0	11	12	0	13	7	9	17	14	0	0	0	10	12	0	18	0
Cristobalite	0	19	0	0	19	0	13	10	0	0	0	0	20	0	0	0	0	0
Albite	9	5	7	7	0	7	8	6	7	7	0	7	5	8	0	6	0	5
Andesine	10	0	3	0	0	3	0	3	6	3	9	3	0	0	0	4	0	0
Oligoclase	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	11
K-feldspar	10	6	9	8	5	7	7	8	5	7	7	6	4	9	3	8	0	3
Calcite	0	2	3	3	0	0	0	1	0	2	0	0	0	2	3	0	4	0
Dolomite	0	0	0	0	35	0	0	2	3	0	3	2	0	0	75	0	70	2
Pyrite	0	2	3	2	1	2	2	2	0	2	0	1	2	3	1	2	0	0
Bulk Subtotal	*67*	*91*	*75*	*74*	*95*	*69*	*76*	*66*	*61*	*69*	*54*	*59*	*94*	*77*	*94*	*63*	*92*	*65*
Clay Minerals																		
Kaolinite	5	5	9	8	4	9	9	9	11	8	14	12	4	8	0	12	0	12
Chlorite	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Illite/smectite	25	4	16	18	1	22	15	25	28	23	32	29	2	15	6	25	8	23
Clay Subtotal	*33*	*9*	*25*	*26*	*5*	*31*	*24*	*34*	*39*	*31*	*46*	*41*	*6*	*23*	*6*	*37*	*8*	*35*
Sample total	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100

[a] Most representative mineral composition for Reef Ridge Shale selected for modeling
g/cm^3 = Grams per cubic centimeter

Table 3. Mineralogy of the Reef Ridge Shale
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Mineral Constituent	Relative Abundance (%)																	
Depth (feet)	*5,356.0*	*5,361.1*	*5,364.6*	*5,371.0*	*5,380.6*	*5,381.0*	*5,383.3*	*5,386.4*	*5,387.4*	*5,391.4*	*5,398.6*	*5,406.5*	*5,410.9*	*5,416.2*	*5,418.5*	*5,423.6*	*5,433.5*	*5,447.5*
Density (g/cm³)	*2.51*	*2.82*	*2.37*	*2.55*	*2.37*	*2.49*	*2.41*	*2.39*	*2.45*	*2.40*	*2.51*	*2.49*	*2.41*	*2.45*	*2.46*	*2.51*	*2.51*	*2.46*
Bulk Minerals																		
Quartz	16	0	0	0	0	10	0	0	0	0	11	0	0	0	5	0	12	0
Opal-CT	25	0	58	25	58	29	47	52	32	51	28	31	46	44	30	33	26	45
Chert	0	10	0	16	0	0	0	0	7	5	0	13	0	10	0	15	0	13
Cristobalite	0	0	22	0	16	0	17	17	15	16	0	0	16	0	11	0	0	0
Albite	7	0	0	7	7	5	6	7	7	8	6	6	7	8	6	7	6	8
Andesine	5	0	0	2	0	8	0	0	2	0	5	2	0	0	2	0	7	0
Oligoclase	0	0	0	0	0	12	0	0	0	0	0	0	0	0	0	0	0	0
K-feldspar	8	0	9	10	4	8	8	7	7	6	6	7	8	7	8	8	8	6
Calcite	0	2	0	2	1	0	1	1	2	0	2	5	2	0	2	3	0	0
Dolomite	2	81	0	0	0	0	1	0	2	0	2	0	0	0	0	0	0	0
Pyrite	0	1	1	3	0	0	1	1	0	1	0	0	1	0	0	2	0	1
Bulk Subtotal	*63*	*94*	*90*	*65*	*86*	*72*	*81*	*85*	*74*	*87*	*60*	*64*	*80*	*69*	*64*	*68*	*59*	*73*
Clay Minerals																		
Kaolinite	11	0	5	9	5	4	7	6	8	6	14	11	7	9	11.0	7	12	8
Chlorite	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Illite/smectite	26	6	5	26	9	24	12	9	18	7	26	25	13	22	25	25	29	19
Clay Subtotal	*37*	*6*	*10*	*35*	*14*	*28*	*19*	*15*	*26*	*13*	*40*	*36*	*20*	*31*	*36*	*32*	*41*	*27*
Sample total	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100

[a] Most representative mineral composition for Reef Ridge Shale selected for modeling
g/cm^3 = Grams per cubic centimeter

Table 4. Estimated Compositions for Carbon Dioxide Injectate

Gas	Mass Faction (original composition)	Mass Fraction (normalized model input)
Injectate Scenario 1		
Carbon dioxide	0.9921253	0.99352
Nitrogen	0.0064308	0.00644
Hydrogen sulfide	0.0000295	0.00001
Sulfur dioxide	0.0000078	0.00003
Total	0.9985934	1.00
Injectate Scenario 2		
Carbon dioxide	0.9988419	0.9995
Methane	0.0003863	0.0004
Ethane	0.0005330	—
Hydrogen sulfide	0.0001394	0.0001
Total	0.9999007	1.00

Note: The original compositions were normalized to 100% for use as model input. For Scenario 2, the ethane component was excluded, as ethane is not in the model database.

Table 5. Mineralogy Input for PHREEQC Selected for Monterey Formation

PHREEQC Mineral	Chemical Formula	Molar Mass (g/mol)	Input	
			%	mol/L
Quartz	SiO_2	60.08	40	52.93
K-Feldspar (orthoclase)	$KAlSi_3O_8$	278.33	16	4.57
Albite (for plagioclase)	$NaAlSi_3O_8$	263.02	32	9.67
Siderite	$Fe(CO_3)$	115.86	0	0
Pyrite	FeS_2	119.98	1	0.66
Gypsum	$CaSO_4{:}2H_2O$	172.17	1	0.46
Smectite-low-Fe-Mg	$Ca_{0.02}Na_{0.15}K.2Fe^{++}{}_{0.29}Fe^{+++}{}_{0.16}Mg_{0.9}Al_{1.25}Si_{3.75}H_2O$	549.07	2.9	0.42
Illite	$K_{0.6}Mg_{0.25}Al_{1.8}Al_{0.5}Si_{3.5}O_{10}(OH)_2$	389.34	5.6	1.14
Kaolinite	$Al_2Si_2O_5(OH)_4$	258.16	1.1	0.34
Chamosite-7A (for chlorite)	$Fe_2Al_2SiO_5(OH)_4$	664.18	0.4	0.05

Note: Depth = 5,981.5 feet; density = 2.65 grams per cubic centimeter (g/cm^3)
g/mol = Grams per mole
mol/L = Moles per liter

Table 6. Mineralogy Input for PHREEQC Selected for Reef Ridge Shale

PHREEQC Mineral	Chemical Formula	Molar Mass (g/mol)	Input	
			%	mol/L
Quartz (+opal, chert, cristobalite)	SiO_2	60.08	50	277.52
Albite (+andesine)	$NaAlSi_3O_8$	263.02	10	12.68
Anorthite (for oligoclase)	$Na_{0.8}Ca_{0.2}Al_{1.2}Si_{2.8}O_8$	265.42	0	0
K-Feldspar (orthoclase)	$KAlSi_3O_8$	278.33	9	10.78
Calcite	$Ca(CO_3)$	100.09	3	9.995
Dolomite	$CaMg(CO_3)_2$	184.4	0	0
Pyrite	FeS_2	119.98	3	8.34
Kaolinite	$Al_2Si_2O_5(OH)_4$	258.16	9	11.63
Chamosite-7A (for chlorite)	$Fe_2Al_2SiO_5(OH)_4$	664.18	0	0
Illite	$K_{0.6}Mg_{0.25}Al_{1.8}Al_{0.5}Si_{3.5}O_{10}(OH)_2$	389.34	16	13.70

Note: Depth = 5,291.8 feet; density = 2.51 grams per cubic centimeter (g/cm^3)
g/mol = Grams per mole
mol/L = Moles per liter

Table 7. Mineralogical Changes Based on Equilibrium Geochemical Modeling for Monterey Formation with Scenario 1 and Scenario 2 Injectates

Mineral	Mineralogical Content (mol/L)											
	Initial	Final	Delta	Initial	Final	Delta	Initial	Final	Delta	Initial	Final	Delta
Sample	*Injection Zone at 5,981.8 feet*						*Injection Zone at 5,981.8 feet*					
Injection Chemistry	*Scenario 1*						*Scenario 2*					
Pressure (atm)	*23.1*			*221.1*			*23.1*			*221.1*		
Albite	9.67	9.42	–0.25	9.67	9.11	–0.56	9.67	9.43	–0.24	9.67	9.12	–0.55
CH_4(g)	—	—	—	—	—	—	0.00	0	–0.0008	0.008	0	–0.008
CO_2(g)	0.75	0	–0.75	7.17	5.44	–1.73	0.76	0	–0.76	7.24	5.50	–1.74
Chamosite-7A	0.05	0	–0.05	0.05	0	–0.05	0.05	0	–0.05	0.05	0	–0.05
Gypsum	0.46	0.45	–0.006	0.46	0.45	–0.015	0.46	0.41	–0.05	0.46	0.44	–0.02
H_2S(g)	0.000008	1.15	1.15	0.00007	1.15	1.15	0.00014	0	–0.00014	0.0013	1.16	1.16
Illite	1.14	1.18	0.04	1.14	2.19	1.05	1.14	1.91	0.77	1.14	2.19	1.05
K-Feldspar	4.57	4.55	–0.02	4.57	4.01	–0.56	4.57	4.16	–0.41	4.57	4.02	–0.55
Kaolinite	0.34	0.50	0.16	0.34	0	–0.34	0.34	0	–0.34	0.34	0	–0.34
N_2(g)	0.0080	0.0079	–0.00014	0.07	0.07	–0.00014	—	—	—	—	—	—
Pyrite	0.66	0	–0.66	0.66	0	–0.66	0.660	0.657	–0.0026	0.66	0	–0.66
Quartz	52.93	53.46	0.53	52.93	54.90	1.97	52.93	53.94	1.01	52.93	54.88	1.95
SO_2(g)	0.00002	0	–0.00002	0.00015	0	–0.00015	—	—	—	—	—	—
Siderite	0	0.77	0.77	0	0.95	0.95	0	0.22	0.22	0	0.95	0.95
Smectite-low-Fe-Mg	0.42	0.39	–0.03	0.42	0	–0.42	0.42	0.15	–0.27	0.42	0	–0.42

Negative (–) delta value indicates that mineral or gas dissolves into solution, while positive (+) delta value indicates that mineral precipitates from solution.
mol/L = Moles per liter
atm = Atmospheres

Table 8. Mineralogical Changes Based on Equilibrium Geochemical Modeling for Reef Ridge Shale with Scenario 1 and Scenario 2 Injectates

Mineral	Mineralogical Content (mol/L)					
	Initial	Final	Delta	Initial	Final	Delta
Sample	*Confining Zone at 5,291.8 feet*			*Confining Zone at 5,291.8 feet*		
Injection Chemistry	*Scenario 1*			*Scenario 2*		
Pressure (atm)	*221.1*			*221.1*		
Albite	12.68	12.67	–0.0088	12.680	12.690	0.006
Anorthite	0	0	0	0	0	0
CH_4(g)	—	—	—	0.008	0	–0.008
CO_2(g)	7.17	3.92	–3.25	7.24	4.00	–3.24
Calcite	10.00	6.48	–3.52	10.00	6.48	–3.52
Chamosite-7A	0	0	0	0	0	0
Dolomite	0	3.54	3.54	0	3.54	3.54
H_2S(g)	0.00007	0.00545	0.00538	0.0013	0.0093	0.0080
Illite	13.70	0	–13.70	13.7	0	–13.7
K-Feldspar	10.78	19.00	8.22	10.78	19.00	8.22
Kaolinite	11.63	23.28	11.65	11.63	23.27	11.64
N_2(g)	0.07300	0.07302	0.00002	—	—	—
Pyrite	8.340	8.337	–0.003	8.34	8.34	–0.000005
Quartz	277.50	277.50	0.019	277.50	277.50	–0.0105
SO_2(g)	0.00015	0	–0.00015	—	—	—

Negative (–) delta value indicates that mineral or gas dissolves into solution, while positive (+) delta value indicates that mineral precipitates from solution.
mol/L = Moles per liter
atm = Atmospheres

Table 9. Modeled Equilibrium Aqueous Concentrations with Scenario 1 and Scenario 2 Injectates

Constituent	Concentration (mg/L[a])					
Geologic Zone	*Monterey Formation at 5,981.5 feet*				*Reef Ridge Shale at 5,291.8 feet*	
Injection Chemistry	*Scenario 1*		*Scenario 2*		*Scenario 1*	*Scenario 2*
Pressure (atm)	*23.1*	*221.1*	*23.1*	*221.1*	*221.1*	
Al^{3+}	0.011	0.0077	0.0104	0.0077	0.0068	0.035
Ba^{2+}	60	60	58	60	72	23
TIC	757	37,127	25,205	37,602	27,819	25,511
Ca^{2+}	386	1,037	2,358	1,086	18	15
Cl^{-}	11,996	11,971	11,667	11,968	14,503	22,826
Fe^{2+}	1.7	0.88	0.57	0.86	212	0.97
K^{+}	243	353	221	349	455	274
Mg^{2+}	472	2,878	1,242	2,907	0.93	0.81
N_2	7.9	7.9	—	—	7.9	—
Na^{+}	15,222	23,818	15,426	23,611	29,105	118,826
SO_4^{2-}	18,203	19,731	6,634	19,049	24,005	6,464
SiO_2	24	25	25	25	24	0
TDS (sum)	47,373	97,008	62,836	96,657	96,222	173,941
pH (s.u.)	6.4	6.3	6.5	6.3	6.1	6.1
pe (unitless)	–2.5	–2.5	–2.9	–2.6	–2.2	–2.4

[a] Unless otherwise noted
mg/L = Milligrams per liter
atm = Atmospheres
TDS = Total dissolved solids
s.u. = Standard units